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~~Our results concern~~ mathematical theory, computational methods, and statistical modeling of chaotic mixing processes.

In mathematical theory, ~~we~~ the authors have proposed a new paradigm for uniqueness and regularization of discontinuous solutions of hyperbolic conservation laws. Contrary to common opinion, there is no requirement from physics for uniqueness of solutions for these systems. Nonuniqueness, if it occurs, must be resolved as in bifurcation theory by an unfolding of critical bifurcation parameters. CONT'D over

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20. ABSTRACT CONTINUED

Similarly regularization does not have to be accomplished by higher order terms in an equation, but may be based on enlarging the system. Many common mathematically based entropy conditions have been shown to be inadequate in specific examples.

Work is in progress on two dimensional nonlinear wave interactions, from a theoretical point of view. Computationally, several difficult phenomena were encountered in the study of shock waves interacting with a liquid-gas interface. This problem produces a reflected rarefaction wave due to the stiff equation of state in water, a transition to an anomolous reflection (related to Mach reflections) and a further transition to a shadow zone of zero propogated signal. There may also be a transition to a vacuum region in the relaxation wave. It appears that front tracking will be superior to other methods for this problem by orders of magnitude, perhaps a factor of 10^5.

Chaotic mixing due to a Rayleigh-Taylor or Richtmyer-Meshkov unstable interface has been studied. Front tracking has provided a unique computational tool, and has produced a unique data set of computational results which are presently being analyzed. High quality models for single-mode growth in the large amplitude regime have been proposed, and validated. These models are correct only for gross flow features, and work on models with validity at a more detailed flow level has been started. The overall goal is to understand chaotic mixing, and considerable progress has been made in this direction.

(KR)

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COMPUTATIONAL TECHNIQUES FOR SHOCK WAVE DIFFRACTION PROBLEMS

FINAL REPORT

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Computational Techniques for Shock Wave Diffraction Problems

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1. Forward

Front tracking is a computational method especially suited to discontinuities such as shock waves and material boundaries. Under research supported by the ARO and detailed in this report, this method has been developed and major obstacles have been overcome. The primary difficulty with front tracking is complexity. We have proved that complex problems, involving many tracked waves and many types of wave interactions, can be handled by this method. New developments in mathematical theory were required, and hence inspired, by front tracking. Applications of this method were to the study of chaotic fluid mixing and interface instability. Progress attained in this area would have been essentially impossible by other computational methods.

2. Table of Contents

3. List of Appendices

There are no appendices to this report.

4. Body of Report

4. A. Statement of the Problem Studied.

The main problem studied was the diffraction and multidimensional interactions of nonlinear hyperbolic waves and fluid discontinuities.

The study includes (a) theoretical and mathematical analysis, (b) development of effective computational methods, especially front tracking methods and (c) scientific studies of wave interactions and chaotic fluid mixing.

4. B. Summary of the Most Important Results.

The central result of the research reported here is that front tracking can be applied and has been developed as a computational method for high resolution computations of fluid discontinuities in two space dimensions, for problems of moderate to high complexity [2,3,11,12,14,16,17,24,25,27]. At the time the research was initiated, such a result was regarded as unattainable.

Many subsidiary results, of considerable interest for their own sake, were obtained in the process of developing front tracking. A remarkable blossoming in mathematical theory for the interaction of nonlinear hyperbolic waves (Riemann problems) has occurred [8-10, 13, 18, 20, 21, 23]. Considerable progress in mathematical modeling of physical phenomena has also been attained [1, 2, 4, 5, 11, 17, 24-26, 28] . Moreover, a deeper understanding of chaotic mixing and unstable interfaces has been achieved [1, 4, 6, 7, 14, 15, 19, 22].

Examples of the mathematical theory include a classification of two dimensional elementary waves [11], the analysis of curvature dependence in the detonation wave speed [1], and the formulation of a conceptual structure for the discussion of higher dimensional Riemann problems [9, 10, 20]. An apparently new wave interaction bifurcation was identified in the analysis of a shock wave passing through a bubble of gas immersed in a liquid [26, 28].

One example of improved mathematical modeling was the discovery that the common mathematical analyses of metastable phase transitions are inconsistent with theoretical and experimental physics [18]. Improved modeling procedures and equations were proposed and related to the literature of theoretical and and experimental physics. Another example of improved modeling concerns entropy conditions to give uniqueness of solutions for Riemann problems. Standard entropy conditions have been shown to be deficient [21]. The correct cure to this disease is not fully understood, but the viscosity method appears to be the most fundamental of the common entropy criteria. Contrary to common opinion, fundamental considerations of physics do not require uniqueness for solutions of the Riemann problem.

Significant progress has been made in the numerical resolution of tracked wave interactions, both for the case of scalar (contact discontinuity) type waves [17], and the interaction of shock waves with material interfaces [24-28]. Other striking examples of improved mathematical modeling associated with front tracking (not funded in the research reported here) can also be listed. The formulation of the laws of elastic deformation in an Eulerian purely conservative form can be mentioned. An analysis of the relation between real fluid equation of state properties and the structure of hydrodynamic waves is another example.

A study of chaotic mixing and unstable interfaces has been made possible by the computational power of front tracking [6,7,15,19,22]. This method is apparently unique in its ability to predict from first principles computations, correct Rayleigh-Taylor mixing zone growth rates over a range of Atwood numbers and compressibilities. Detailed analysis of laboratory experiments has produced some surprises. Carefully computed and validated single mode theories are not applicable to chaotic flow regimes [19]. A superposition hypothesis has some power in explaining the influence of neighboring modes on a leading bubble in the growing mixing zone [22]. Simple three and four parameter models of the single bubble mode were developed and shown to be valid over all time periods: exponential growth, uniform acceleration and approach to terminal velocity. This theory is one of the ingredients to the superposition analysis of chaotic flows regimes.

A major observation from experiments has been the almost universal aspect of the growth of the mixing zone. Our research indicates that universality is not due to the large number of bubble mergers, leading to a loss of dependence on initial conditions. Rather a better explanation seems to be the existence of a thermodynamic limit, or ensemble average, due to the presence of a large number of bubbles in the spatial array. In other words, space averages rather than time averages appear to be the dominant mechanism.

In summary, the research supported by the ARO has led to the establishment of front tracking as an accurate and efficient computational method that can be applied to a variety of problems where discontinuities are important. The requirements of this method provide a dynamic feedback to the mathematical theory and thus lead to a better understanding of the underlying theory. The work initiated with the ARO's support has developed into an ongoing effort in scientific computing, and will continue to produce new and improved theory and computation in the future.

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4. D. Participating Scientific Personnel

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